



# “X-ray and neutron diffraction studies of macromolecules: from data collection to structures”

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*AN INTERNATIONAL iNEXT, UNIOGS-HEALTH AND BIOSCIENCES DOCTORAL PROGRAMME, BIOCENTER OULU, AND BIOCENTER FINLAND COURSE*

*FACULTY OF BIOCHEMISTRY AND MOLECULAR MEDICINE,*

*UNIVERSITY OF OULU, FINLAND*

May 15 – 19, 2017



**iNEXT**



**BF**  
BioCenter Finland

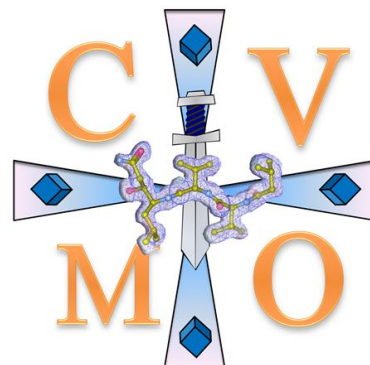
## Collaborators



Finnish Synchrotron Radiation  
Users Organization



## Sponsors and funding sources



- All events are in the FBMM building on the Kontinkangas campus (first floor)
- Coffee is available (20/30-Euro cents per cup, bring your own cup) in the FBMM cafeteria (2 floor)
- The full course will provide 2 ECTS credits. The 15 lectures (highlighted in yellow) can be attended also by researchers who are not participating in the tutorials. When attending all lectures a 1 ECTS certificate will be provided. All lectures are in F101 (FBMM).

## Monday, May 15

08:30 Pickup by bus from the hotel to Aapistie 7 A

*Chair person: Rik Wierenga*

09:00 Welcome (F101) Rik Wierenga (general), Johanna Myllyharju (welcome from Biocenter Oulu), Lari Lehtiö (computing), Kristian Koski (remote data collection)

09:30-10:15 Bernhard Rupp (Vista, USA)

**Dectris Lecture (F101) "Basic concepts of biomolecular crystallography, part-I"**

10:15-10:45 Coffee/Tea (F101)

10:45-11:30 Bernhard Rupp (Vista, USA)

**Dectris Lecture (F101) "Basic concepts of biomolecular crystallography, part-II"**

11:30-12:15 Marjolein Thunnissen (MAX IV, Lund, Sweden)

**Lecture (F101) "Datacollection at synchrotrons"**

12:15-13:15 Lunch, Restaurant Medisiina

*Chair person Lari Lehtiö*

13:15-14:00 Armin Wagner (Diamond, Oxford, UK)

**Lecture (F101) "Benefits and perspectives of the long wavelength beam line at Diamond"**

14:00-14:45 Esko Oksanen (ESS, Lund, Sweden)

**Lecture (F101) "Neutron diffraction from single macromolecular crystals: sample preparation and beam lines"**

14:45-15:15 Coffee/Tea/Cake (F101)

*Chair person: Lari Lehtiö*

15:15-16:45 Student talks (F101)

16:45-17:45 Startup of the Linux class room (Lari, Ari-Pekka)

18:00 Dinner, Restaurant Kastellin tutkimuskeskus (Kontinkangas campus)

19:00 Bus transportation back to hotel from Restaurant Kastellin Tutkimuskeskus

## Tuesday, May 16

08:30 Pickup by bus from the hotel to Aapistie 7 A

*Chair person: Tiila-Riikka Kiema*

09:00-09:45 Andrey Lebedev (CCP4, STFC, Harwell campus, Oxford, UK)  
Lecture (F101) "Molecular replacement"

09:45-10:30 Esko Oksanen (ESS, Lund, Sweden)  
Lecture (F101) "Neutron data processing protocols"

10:30-10:45 Coffee/Tea (F101)

*Chair person: Gabriele Cordara*

10:45-11:30 Bernhard Rupp (Vista, USA)  
Lecture (F101) "The PDB validation report"

11:30-13:00 Bernhard Rupp (Vista, USA)  
Tutorial (F132) "The PDB validation tutorial" (Gabriele, Deborah, Rik)

13:00-14:00 Lunch, Restaurant Medisiina

*Chair person: Kristian Koski*

14:00-14:45 Karine Rower (BESSY, Berlin, Germany)  
Lecture (F101) "Data processing by XDS"

14:45-15:30 David Waterman (CCP4, STFC, Harwell campus, Oxford) (F101)  
Lecture (F101) "Data processing by DIALS"

15:30-15:45 Coffee/Tea/Cake (F132)

15:45-17:45 Andrey Lebedev (CCP4, STFC, Harwell campus, Oxford, UK)  
Tutorial (F132) "Molecular replacement tutorial" (Tiila, Shiv)

18:00 Dinner, Restaurant Kastellin tutkimuskeskus (Kontinkangas campus)

19:00 Bus transportation back to hotel from Kastellin tutkimuskeskus (Kontinkangas campus)

## Wednesday, May 17

08:30 Pickup by bus from the hotel to Aapistie 7 A

09:00-11:00 Karine Rower (BESSY, Berlin, Germany)  
tutorial "XDS" (F132) (Katja, Abhi, Ezeogo)

11:00-11:15 Coffee/Tea (F132)

11:15-13:15 David Waterman (CCP4, STFC, Harwell campus, Oxford, UK)  
tutorial "DIALS" (F132) (Kristian, Tiila, Harry Powell)

13:15-14:15 lunch, Restaurant Medisiina

*Chair person: Mirko Maksimainen*

14:15-15:00 Anne Tuukkanen (EMBL Hamburg, Germany)  
Lecture (F101) "Insights from SAXS and SANS experiments in structural biology research"

15:00-15:45 Tim Gruene (SLS-PSI, Villigen, Switzerland)  
Lecture (F101) "SHELX for experimental phasing and refinement"

15:45-16:00 Coffee/Tea/Cake (F132)

16:00-17:45 Bernhard Rupp (Vista, USA)  
Tutorial (F132) "Validation" (Gabriele, Deborah, Rik)

18:00 Bus transportation to Flying Reindeer, in city center of Oulu

## Thursday, May 18

08:30 Pickup by bus from the hotel to Aapistie 7 A

*Chair person: Tiila Kiema*

09:00-09:45 Alberto Podjarny (IGBMC, Strassburg, France)

Lecture (F101) "New insights from atomic structures obtained from neutron crystallography"

09:45-09:50 Photograph

09:50-10:00 Coffee/Tea (F132)

10:00-12:00 Esko Oksanen (ESS, Lund, Sweden)

Tutorial (F132) "Neutron scattering refinement using Phenix" (Lari, Mirko)

12:00-13:00 Lunch, Restaurant Medisiina

13:00-15:00 Tim Gruene (SLS-PSI, Villigen, Switzerland)

Tutorial (F132) "Experimental phasing SHELX C/D/E" (F132) (Mirko, Gabriele)

15:00-15:15 Coffee/Tea/Cake (F132)

15:15-16:00 Bernhard Rupp (Vista, USA)

Tutorial (F132) "Validation" (Gabriele, Deborah, Rik)

16:00-17:45 (F132) Students can work with their own data (all teachers)

18:00 Dinner, Restaurant Kastellin tutkimuskeskus (Kontinkangas campus)

19:00 Bus transportation back to hotel from Kastellin tutkimuskeskus (Kontinkangas campus)

## Friday, May 19

08:30 Pickup by bus from the hotel to Aapistie 7 A

*Chair person: Rik Wierenga*

09:00-10:00 Janos Hajdu (University of Uppsala, Uppsala, Sweden) (F101)  
Lecture (F101) "Basic principles of the XFEL-technique and its structural biology perspectives"

10:00-10:30 Coffee/Tea (F101)

*Chair person: Gabriele Cordara*

10:30-11:30 Pierre Aller (Diamond, Oxford, UK)  
Lecture (F101) "The Diamond protein crystallography beam lines"

11:30-12:15 Harry Powell (Diamond, Oxford, UK)  
Lecture (F101) "How to use the synchrotron data processing pipelines"

12:15-13:15 Lunch, Restaurant Medisiina

13:15-14:15 Pierre Aller (Diamond, Oxford, UK)  
Demonstration (F121A) Remote data collection demonstration with test crystals (group-1) (Kristian, Tiila, Gabriele)

13:15-14:15 Ed Daniel (University of Oulu, Oulu, Finland)  
Demonstration (F132) IceBear demonstration (group-2) (Rik)

14-15:14:30 Coffee/Tea/Cake (F132)

14:30-15:30 Pierre Aller (Diamond, Oxford, UK)  
Demonstration (F121A) Remote data collection demonstration with test crystals (group-2) (Kristian, Tiila, Gabriele)

14:30-15:30 Ed Daniel (University of Oulu, Oulu, Finland)  
Demonstration (F132) IceBear demonstration (group-1) (Rik)

15:30- Pierre Aller, Harry Powell (Diamond, Oxford, UK)  
Data collection (F121A). Remote data collection from own crystals (Kristian, Tiila, Gabriele, Mirko, Katja)

15:30- (F132) Students work in the Linux class room

18:00 Final get-together with snacks (FBMM cafeteria)  
Student-presentation prize (Bernhard Rupp)

19:00 Bus transportation back to the hotel from Aapistie 7 A